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RESEARCH MEMORANDUM

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ABSTRACT

Response variances $\mathrm{var}(y_i)$ are estimated from m replications per experimental condition. The resulting estimated variances s_i^2 can be used to derive the correct variances of the Ordinary Least Squares (OLS) estimators $\hat{\beta}$. The estimates s_i^2 can also be used to compute the Estimated Weighted Least Squares (EWLS) estimators $\hat{\beta}^*$. The asymptotic covariance formula for EWLS might be utilized to test these estimators $\hat{\beta}^*$. The type I and type II errors of this test procedure are compared to the corresponding errors of the OLS test.

1. INTRODUCTION

This paper is a continuation of Kleijnen, Brent and Brouwers (1981) and Nozari (1984); also see Deaton, Reynolds and Myers (1983). The problem we face is: we have the classical general linear model

$$\underset{\sim}{y} = \underset{\sim}{X} \cdot \underset{\sim}{\beta} + \underset{\sim}{e} \tag{1.1}$$

but the errors $\underset{\sim}{e}$ may show strong <u>heterogeneity of variance</u>. We have variance estimators s_i^2 based on replicating the experimental conditions i, say m_i times:

$$s_i^2 = \sum_{j=1}^{m_i} (y_{ij} - \bar{y}_i)^2/(m_i-1) \qquad (i = 1,\dots,n) \tag{1.2}$$

We examine the following questions:

(1) Are Ordinary Least Squares (OLS) robust? So we compute

$$\hat{\underset{\sim}{\beta}} = (\underset{\sim}{X}'.\underset{\sim}{X})^{-1}.\underset{\sim}{X}'.\underset{\sim}{y} \tag{1.3}$$

and

$$\underset{\sim}{\Omega}_{\hat{\beta}} = (\underset{\sim}{X}'.\underset{\sim}{X})^{-1}.\sigma^2 \tag{1.4}$$

$$\hat{\sigma}^2 = \sum_{i=1}^{n}\sum_{j=1}^{m_i} (y_{ij} - \hat{y}_{ij})^2/(N-q) \tag{1.5}$$

where q denotes the number of parameters, $N = \sum_{i=1}^{n} m_i$ and $\hat{y}_{ij} = \hat{y}_i$. The classical t statistic with $v = N-q$ degrees of freedom is:

$$t_v = \frac{\hat{\beta}_j - \beta_j}{\{\widehat{\mathrm{var}}\,(\hat{\beta}_j)\}^{\frac{1}{2}}} \qquad (j = 1,\dots,q) \tag{1.6}$$

(2) Can we use the OLS estimator $\hat{\underset{\sim}{\beta}}$ of (eq. 1.3) combined with the <u>correct</u> expression for the <u>covariance matrix</u> $\underset{\sim}{\Omega}_{\hat{\beta}}$ in case of unequal variances? Obviously we have:

$$\Omega_{\hat{\beta}} = (\underset{\sim}{X}'.\underset{\sim}{X})^{-1}.\underset{\sim}{X}'.\underset{\sim}{\Omega}_y.\underset{\sim}{X}.(\underset{\sim}{X}'.\underset{\sim}{X})^{-1} \tag{1.7}$$

We can estimate Ω_y using s_i^2 of eq. (1.2). But how many degrees of freedom has the t statistic of eq. (1.6)? It is easy to derive that eq. (1.3) reduces to

$$\hat{\beta}_j = \sum_{i=1}^{n} \bar{x}_{ij}.\bar{y}_i/n \qquad (j = 1,\dots,q) \tag{1.8}$$

where $\bar{x}_{ij}$ is the (i,j)th element of the n × q matrix $\bar{\underset{\sim}{X}}$ formed by the n different rows of the N × q matrix $\underset{\sim}{X}$ (remember: $N = \Sigma\, m_i$; m_i replicates), and we restrict this study to experimental designs with $\bar{\underset{\sim}{X}}'.\bar{\underset{\sim}{X}} = n.\underset{\sim}{I}$. Because $(\bar{x}_{ij})^2$ equals plus one, and the observations are independent we obtain:

$$\mathrm{var}\,(\hat{\beta}_j) = \sum_{i=1}^{n} \mathrm{var}\,(\bar{y}_i)/n^2 \tag{1.9}$$

Using the estimator s_i^2 of eq. (1.2) we get:

$$\hat{\mathrm{var}}\,(\hat{\beta}_j) = \sum_{i=1}^{n} (s_i^2/m_i)/n^2 \tag{1.10}$$

We further restricted our study to equal numbers of replications (m_i = m) so that $\hat{\mathrm{var}}\,(\hat{\beta}_j)$ reduces to a sum of χ^2 variates. Because of the additivity of χ^2 variates the t statistic of eq. (1.6) has degrees of freedom $v = n.(m-1)$.

<u>Note</u>: If $m_i \neq m$ then we would recommend $m_i = c\ \hat{\mathrm{var}}\,(y_{ij})$ so that $\mathrm{var}\,(\bar{y}_i)$ is (approximately) constant.

(3) Can we use the variance estimators s_i^2 in <u>Estimated Weighted Least Squares</u> (EWLS)? Or

$$\hat{\underset{\sim}{\beta}}^* = (\bar{\underset{\sim}{X}}' . \hat{\bar{\underset{\sim}{\Omega}}}_y^{-1} . \bar{\underset{\sim}{X}})^{-1} . \bar{\underset{\sim}{X}}' . \hat{\bar{\underset{\sim}{\Omega}}}_y^{-1} . \bar{\underset{\sim}{y}} \tag{1.11}$$

The <u>asymptotic</u> covariance matrix of EWLS is:

$$\hat{\underset{\sim}{\Omega}}_{\hat{\beta}^*} = (\bar{\underset{\sim}{X}}' . \hat{\bar{\underset{\sim}{\Omega}}}_y^{-1} . \bar{\underset{\sim}{X}})^{-1} \tag{1.12}$$

Eqs. (1.11) and (1.12) result in the analogue of the t statistic of eq. (1.6). However, it is more difficult to determine the correct degrees of freedom v^*. We might investigate:

(i) $v^* = N - q = n.m - q$; see the classical OLS formulas.

(ii) $v^* = \sum_{1}^{n} (m_i - 1) = n.(m-1) = n.m - n$; see eq. (1.10).

(iii) $v^* = \min_i (m_i - 1) = m-1$; see Scheffé (1964).

(iv) $v^* = \infty$ or $t_v = z$ with $z \sim N(0,1)$; the asymptotic case.

Actually we did not investigate approach (i). One reason is that approach (i) assumes a correctly specified regression model whereas the other approaches use the unbiased estimators s_i^2. The difference between (i) and (ii) is minor if $q \quad n$ (with $q \leq n$).

2. MONTE CARLO INPUT PARAMETERS

The parameters of our Monte Carlo experiment are as follows: All $n \times q$ matrices $\bar{\underset{\sim}{X}}$ are orthogonal. One $\bar{X}$ is a 16×13 matrix $\bar{\underset{\sim}{X}}$ taken from a simulation study on the Rotterdam harbor (with design generators $\underset{\sim}{1} = \underset{\sim}{5}.\underset{\sim}{6}$ and $\underset{\sim}{3} = \underset{\sim}{4}.\underset{\sim}{5}$) and corresponding β vector; see Kleijnen et al. (1981; note 3). The other matrices $\bar{\underset{\sim}{X}}$ are 8×4 and 4×3 respectively. We combine each of these three cases with several degrees of heterogeneity measured by

$$H = (\sigma^2_{max} - \sigma^2_{min})/\sigma^2_{min} \tag{2.1}$$

where σ^2_{max} (and σ^2_{min}) is the maximum (and minimum) element of Ω_y. H varies between zero (constant variances) and 1,455.69 (taken from the harbor study). The variances are estimated from m replications where we varied m between two (a technical minimum) and twenty-five.

We repeated each Monte Carlo experiment (specified by $\bar{\underset{\sim}{X}}$, $\underset{\sim}{\beta}$, $\underset{\sim}{\Omega}_y$, and m) 150 times to reduce chance effects. We used a multiplicative random number generator with multiplier 13^{13} and modulus 2^{59}. This generator was developed by NAG (Numerical Algorithms Group) and it is standard on our ICL 2960 computer.

3. MONTE CARLO RESULTS

In Appendix 1 we present the results that substantiate the experimental results of Kleijnen et al. (1981). In other words we repeat the experiment of Kleijnen et al. (1981) with different random numbers and find the following results:

(i) Bias: OLS gives unbiased estimators $\hat{\underset{\sim}{\beta}}$ as we knew, and EWLS gives unbiased estimators $\hat{\underset{\sim}{\beta}}^*$ too.

(ii) Standard errors: The asymptotic covariance formula of eq. (1.12) applies if we estimate var (y) from twenty-five replications (m = 25). For m = 9 our results deviate from Kleijnen et al. (1981): the asymptotic formula may very well underestimate the variance.

(iii) Relative efficiency: In case of strong heterogeneity EWLS gives smaller variances for the β estimators provided we have more than two replications ($m > 2$).

Next we try to answer a new set of questions, namely can we use the Student t statistic t_v when we estimate the unknown variances $\mathrm{var}\ (\bar{y}_l)$ and apply OLS and EWLS respectively, where the degrees of freedom v may equal $n(m-1)$ for OLS and $(m-1)$, $n(m-1)$ or ∞ for EWLS. We estimate the true distribution from 150 realizations, and apply three popular goodness-of-fit tests, namely the χ^2, the Kolmogorov-Smirnov, and the Anderson-Darling test. We apply each goodness-of-fit test to each of the q parameters β_j, with a 1% significance level. We do not present the mass of data but report our preliminary results (which are further investigated below): EWLS based on only two replications result in distributions not well approximated by any Student distribution. If we have more replications ($m > 2$) then we may use the Student t statistic with the (conservative) degrees of freedom equal to $m-1$. If m is as high as 25 then we may use the normal approximation. OLS with the corrected variance formula accounting for unequal variances (eq. 1.7) results in a t distribution with degrees of freedom equal to $n(m-1)$, provided $n(m-1) > 15$ (as n increases the variance of $\widehat{\mathrm{var}}\ (\hat{\beta})$ decreases). We shall give more detailed results for the following more specialized question.

Because we use the t distribution only to select the critical constant $t_v^{\alpha/2}$, we test the hypothesis:

$$H_0\ :\ P\left\{\frac{|\hat{\beta}_j - \beta_j|}{\{\widehat{\mathrm{var}}\ (\hat{\beta}_j)\}^{\frac{1}{2}}} > t_v^{\alpha/2}\right\} = \alpha \qquad (j = 1,\ldots,q) \tag{3.1}$$

versus the alternative hypothesis $H_1\ :\ P\{e\} \neq \alpha$ or the one-sided and conservative alternative hypothesis $H_1\ :\ P\{e\} > \alpha$, where e denotes the event within the brackets of eq. (3.1). To test H_0 we use the binomial test as follows. We estimate $P\{e\}$ from 150 independent replications and compute a confidence interval. For example, for the one-sided H_1 the lower limit of the $1-\gamma_0$ confidence interval is given by the following expression where z^{γ_0} is defined by $P(z > z^{\gamma_0}) = \gamma_0$ and $z \sim N(0,1)$:

$$\hat{p}-z^{\gamma_0}.\{\hat{p}.(1-\hat{p})/150\}^{\frac{1}{2}} \tag{3.2}$$

We reject H_0 if α is smaller than this limit. We reject H_0 if for any of the q parameters β_j we exceed the critical level: Applying the Bonferroni inequality we reject H_0 if:

$$\max_{1 \leq j \leq q} [\hat{p}_j - z^{\gamma/q} . \{\hat{p}_j . (1-\hat{p}_j)/150\}^{\frac{1}{2}}] > \alpha \qquad (3.3)$$

We fix γ in eq. (3.3) at 5%. We apply this procedure for three classical α values in eq. (3.1), namely 1%, 5% and 10%. This approach results in Tables I and II where the symbol * means that we reject H_0. These tables suggest the following conclusions: If the n responses $\bar{y}$ have different variances and we can estimate these variances from more than two replications ($m > 2$) then the OLS estimators $\hat{\beta}$ can be tested using a Student t statistic with degrees of freedom equal to $v = n(m-1)$, provided we test β with an α exceeding 1%. Testing the EWLS estimators $\hat{\beta}^*$ requires more replications, say $m = 25$ (and $\alpha > 0.01$). This conclusion agrees with Nozari (1983)'s conclusion.

If both OLS and EWLS result in (roughly) the same α error then we may proceed to a comparison of their power functions. We estimated the power function in a few points (from eight to ten points) using different random numbers per point. (In Kleijnen (1984) we shall present a more efficient procedure.) For each point we generate 150 replicates. In all experiments the estimated power of EWLS dominated that of OLS (as we might expect because in previous experiments we found that $\mathrm{var}(\hat{\beta}^*) < \mathrm{var}(\hat{\beta})$) which we tested through the sign test.

4. CONCLUSIONS

If we suspect heterogeneity of variances then we should try to estimate the n different variances, using more than two replications ($m > 2$). We can use these estimated variances to derive the correct variances of the OLS estimators $\hat{\beta}$ and to test their significance, through the Student t statistic with $n(m-1)$ degrees of freedom. If we have firm estimators of the response variances - say 25 replications - then it is better to use the EWLS estimators $\hat{\beta}^*$ with the t distribution with degrees of freedom equal to $n(m-1)$. We should test OLS and EWLS estimators using an α higher than 1%.

TABLE I

Testing the tail of the t_v distribution; one-sided test

	α = 1%				α = 5%				α = 10%			
	OLS	EWLS			OLS	EWLS			OLS	EWLS		
	$t_{n(m-1)}$	t_{m-1}	$t_{n(m-1)}$	t_∞	$t_{n(m-1)}$	t_{m-1}	$t_{n(m-1)}$	t_∞	$t_{n(m-1)}$	t_{m-1}	$t_{n(m-1)}$	t_∞
C1H11m2			*	*			*	*			*	*
C1H1455m2			*	*	*		*	*	*		*	*
C2H10m2			*	*			*	*			*	*
C2H1455m2			*	*	*		*	*	*	*	*	*
C3H10m4			*	*			*	*			*	*
C3H1289m4			*	*			*	*			*	*
C3H10m5				*				*				*
C3H1289m5			*	*			*	*			*	*
C1H0m9							*	*			*	*
C1H11m9												
C1H1455m9												
C2H0m9												
C2H10m9			*	*			*	*			*	*
C2H1455m9				*			*	*			*	*
C3H10m9												
C3H1289m9			*	*			*	*	*	*	*	*
C1H0m25												
C1H11m25												
C1H1455m25												
C2H0m25												
C2H10m25												
C2H1455m25												
C3H10m25												
C3H1289m25												

C1H11m2 means: Case 1 (n = 16, q = 13), Heterogeneity factor H = 11, replications m = 2. Etc.

TABLE II

Testing the tail of the t_v distribution; two-sided test

	α = 1%				α = 5%				α = 10%			
	OLS	EWLS			OLS	EWLS			OLS	EWLS		
	$t_{n(m-1)}$	t_{m-1}	$t_{n(m-1)}$	t_∞	$t_{n(m-1)}$	t_{m-1}	$t_{n(m-1)}$	t_∞	$t_{n(m-1)}$	t_{m-1}	$t_{n(m-1)}$	t_∞
C1H11m2	*	*	*	*		*	*	*		*	*	*
C1H1455m2		*	*	*	*	*	*	*		*	*	*
C2H10m2		*	*	*		*	*	*			*	*
C2H1455m2		*	*	*	*	*	*	*	*		*	*
C3H10m4		*	*	*			*	*			*	*
C3H1289m4				*			*	*			*	*
C3H10m5		*						*				
C3H1289m5		*		*		*	*	*			*	*
C1H0m9	*	*						*		*	*	*
C1H11m9	*	*	*			*						
C1H1455m9	*	*								*		
C2H0m9	*	*										
C2H10m9												*
C2H1455m9		*					*	*			*	*
C3H10m9	*	*				*						
C3H1289m9				*			*	*	*		*	*
C1H0m25	*	*	*	*		*				*		
C1H11m25	*	*	*	*		*	*	*	*	*	*	*
C1H1455m25	*	*	*	*								
C2H0m25	*	*	*	*								
C2H10m25	*	*	*	*								
C2H1455m25	*	*	*									
C3H10m25												
C3H1289m25	*	*	*	*		*						

APPENDIX 1: REPEATING THE EXPERIMENT OF KLEIJNEN ET AL. (1981)

We first check the correctness of our Monte Carlo computer program as follows. We know that the OLS estimator $\hat{\beta}$ of eq. (1.3) or (1.8) is unbiased and that its covariance matrix is given by eq. (1.7) or (1.9) where $\Omega_{\tilde{y}_\alpha}$ or var $(\bar{y})$ is known in the Monte Carlo experiment. So we estimated the expected values $E(\hat{\beta}_j)$ and the variances var $(\hat{\beta}_j)$ from the 150 Monte Carlo repetitions and tested these values using the standard normal z statistic respectively the χ^2 statistic with 149 degrees of freedom.

Next we examine the quality of the various β estimators in several steps:

(i) Bias of β estimator

We know that OLS give unbiased estimators $\hat{\beta}$, and that under mild technical assumptions EWLS also give unbiased estimators $\hat{\beta}^*$. In the preceding paragraph we verified the lack of bias in OLS. For EWLS we computed the (approximate) Student t statistic:

$$t_{149}^{(j)} \quad \frac{\left(\sum_{g=1}^{150} \hat{\beta}_{jg}^*/150\right) - \beta_j}{\left\{\sum_{g=1}^{150} \left(\hat{\beta}_{jg}^* - \sum_{g=1}^{150} \hat{\beta}_{jg}^*/150\right)^2/(149 \times 150)\right\}^{\frac{1}{2}}} \quad (j = 1,\ldots,q) \quad (A.1)$$

Note: We do not use the equality sign in eq. (A.1) because the EWLS estimator $\hat{\beta}^*$ is not a linear transformation of $\bar{\underset{\sim}{y}}$; $\hat{\beta}^*$ also uses the random vector with the elements s_i^2. However, the t statistic is supposed to be robust, especially with as many observations as 150.

We obtain 160 realizations of t_{149} (the number 160 follows from Table III later on). We use a 5% significance level per realization so that we expect eight false significances. We find zero significances for OLS and six for EWLS. We conclude that OLS and EWLS do give unbiased estimators of β which agrees with Kleijnen et al. (1981).

(ii) Standard error of β estimator

The standard errors of the OLS estimators $\hat{\beta}$ follow from eq. (1.7) or eq. (1.10). For EWLS we have the asymptotic formula of eq. (1.12). We compute the χ^2 approximation:

$$\chi^{2(j)}_{149} \quad \frac{\sum_{g=1}^{150} (\hat{\beta}^{*}_{jg} - \sum_{g=1}^{150} \hat{\beta}^{*}_{jg}/150)^2/149}{(\bar{X}'.\hat{\Omega}^{-1}_{\bar{y}}.\bar{X})^{-1}_{jj}} \qquad (j = 1,\ldots,q) \qquad \text{(A.2)}$$

where $(\ )_{jj}$ means the j-th element on the main diagonal of ( ). Table III displays the maximum and the minimum of the q realizations. We compare the maximum and minimum using a two-sided χ^2_{149} test with 1% significance, resulting in the critical values 0.73 and 1.32. Table III suggests the following conclusions. With only two replications (m) to estimate var(y) we underestimate the true variance of $\hat{\beta}^{*}$. With m = 25 the asymptotic formula gives unbiased estimators of var($\hat{\beta}^{*}$). With m = 9 we may very well underestimate the variance; our results for m = 9 conflict with Kleijnen et al. (1981) who reported unbiased estimators.

Note: We use the χ^2 statistic even though $\hat{\beta}^{*}$ may be nonnormal and we know that the χ^2 statistic is not robust. However, we do not apply a distribution-free procedure because we have 149 degrees of freedom and because ultimately we are not interested in the standard errors themselves but in their role when using a t statistic like eq. (1.6); see Section 3.

<u>(iii) Efficiency of OLS versus EWLS</u>

We measure the efficiency by the variance. Therefore we compare the estimated variance of the EWLS estimator (the numerator of eq. (A.2)) to the known variance of the OLS estimator (see eq. (1.9)) which results in a χ^2_{149} statistic analogous to eq. (A.2). Table IV suggests the following conclusions (which agree with Kleijnen et al. (1981)):

(i) If we knew that the variances var($\bar{y}$) are constant (H = 0), then we should not estimate them, i.e., we should not use EWLS.

(ii) In case of strong heterogeneity we should use EWLS provided we can estimate var($\bar{y}$) from more than two observations.

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TABLE III

Adequacy of asymptotic variance formula

Case 1: $n = 16$, $q = 13$

Heterogeneity H

	0		11.84			1,455.69		
m	9	25	2	9	25	2	9	25
max χ^2	1.399*	1.207	1.643*	1.215	1.238	1.792*	1.186	1.224
min χ^2	0.834	0.823	1.013	0.914	0.674*	1.236	0.923	1.005

Case 2: $n = 8$, $q = 4$

Heterogeneity H

	0		10.83			1,455.69		
m	9	25	2	9	25	2	9	25
max χ^2	1.195	1.211	2.427*	1.348*	1.038	3.635*	1.183	0.918
min χ^2	0.948	1.047	1.680	1.074	0.899	2.642	0.947	0.873

Case 3: $n = 4$, $q = 3$

Heterogeneity H

	10.38				1,289.15			
m	4	5	9	25	4	5	9	25
max χ^2	1.251	1.100	1.092	1.120	1.315	1.184	1.399*	1.049
min χ^2	1.169	0.903	0.945	0.962	1.012	0.978	0.993	0.792

TABLE IV

Efficiency of OLS versus EWLS

Case 1: n = 16, q = 13

Heterogeneity H

	0		11.84			1,455.69		
m	9	25	2	9	25	2	9	25
max χ^2	1.399*	1.207	1.453*	1.195	1.217	1.436*	0.949	0.941
min χ^2	0.834	0.823	0.993	0.864	0.673*	0.097*	0.077*	0.075*

Case 2: n = 8, q = 4

Heterogeneity H

	0		10.83			1,455.69		
m	9	25	2	9	25	2	9	25
max χ^2	1.195	1.211	1.827*	1.203	0.989	0.560	0.190	0.162
min χ^2	0.948	1.047	1.389	0.732	0.635*	0.150*	0.052*	0.046*

Case 3: n = 4, q = 3

Heterogeneity H

	10.38				1,289.15			
m	4	5	9	25	4	5	9	25
max χ^2	1.237	1.100	1.017	1.096	1.214	1.119	1.242	0.915
min χ^2	0.763	0.589*	0.684*	0.730	0.352*	0.395*	0.345*	0.275*

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